Figure 1

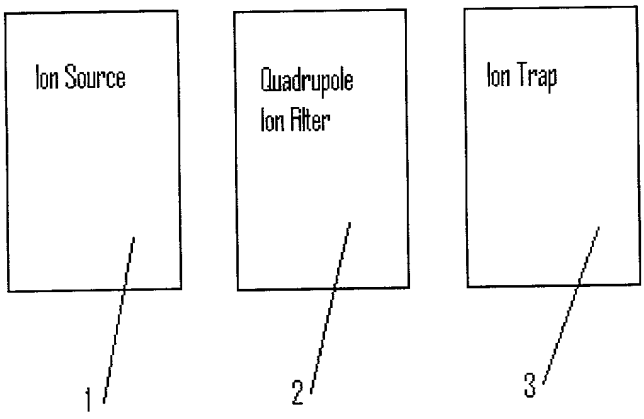

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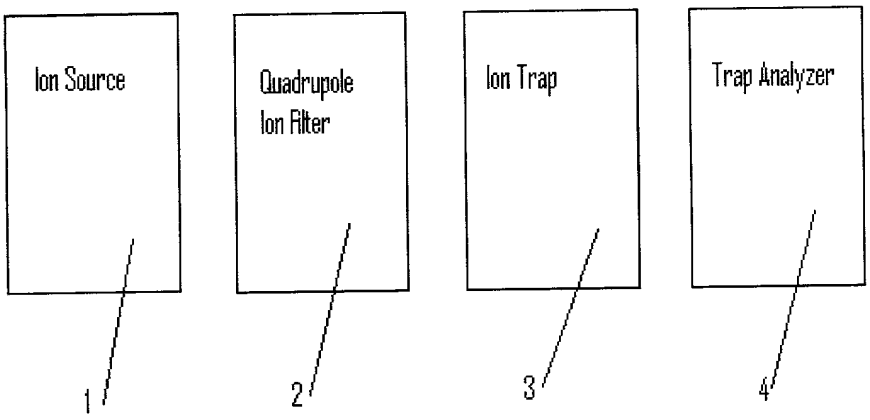
Figure 2



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TO2TOT"5059660

FIGURE 3

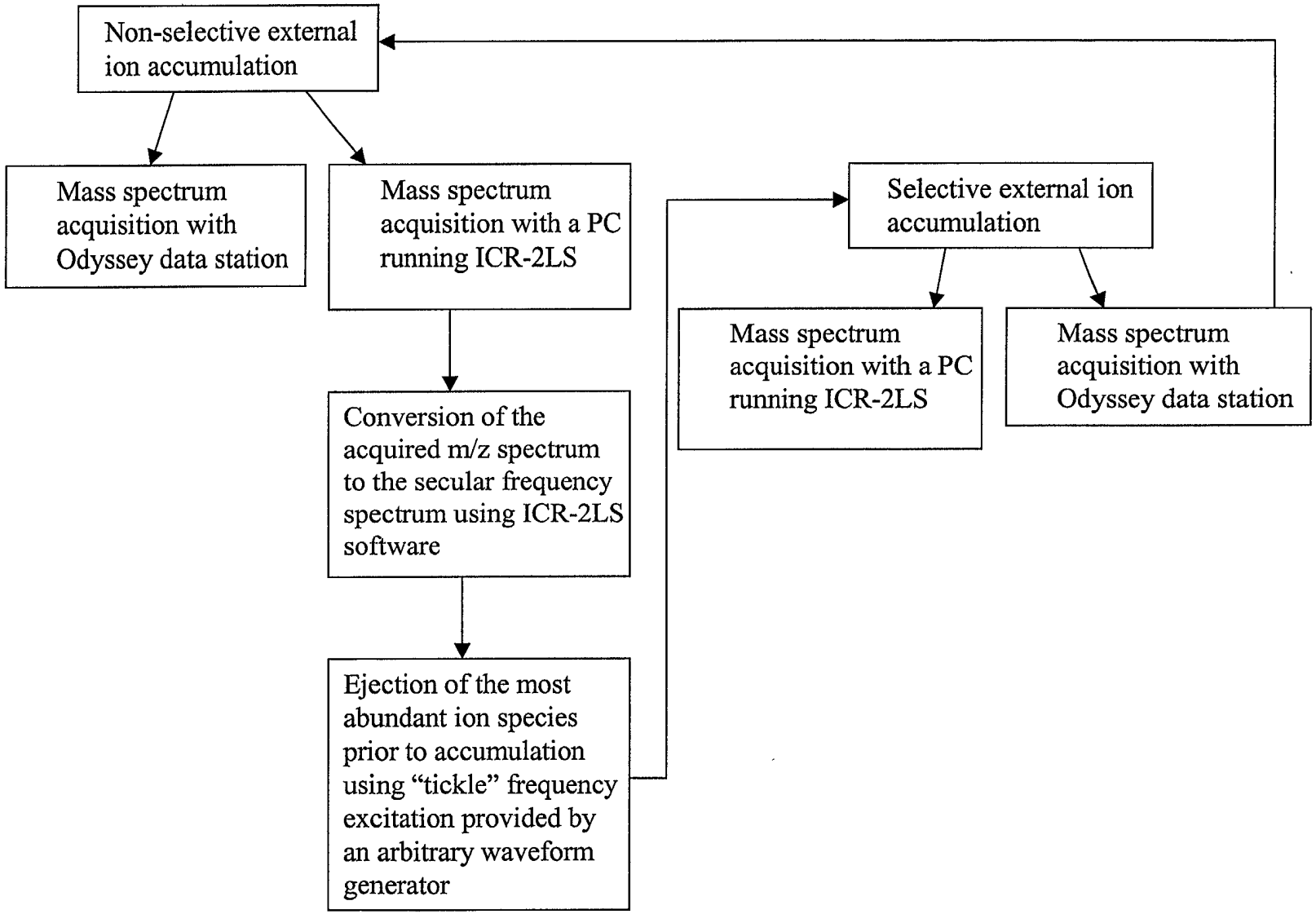


FIGURE 4

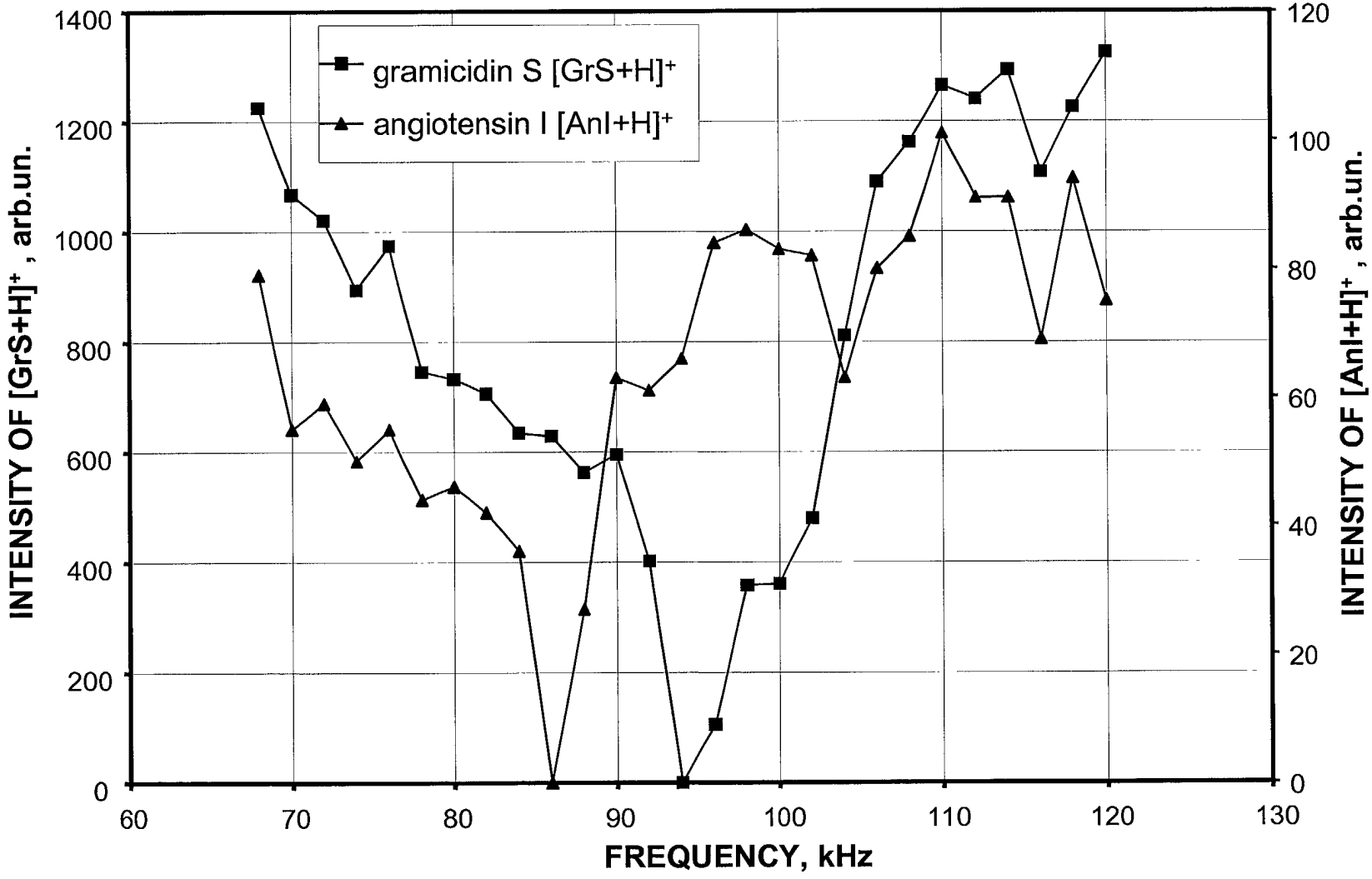
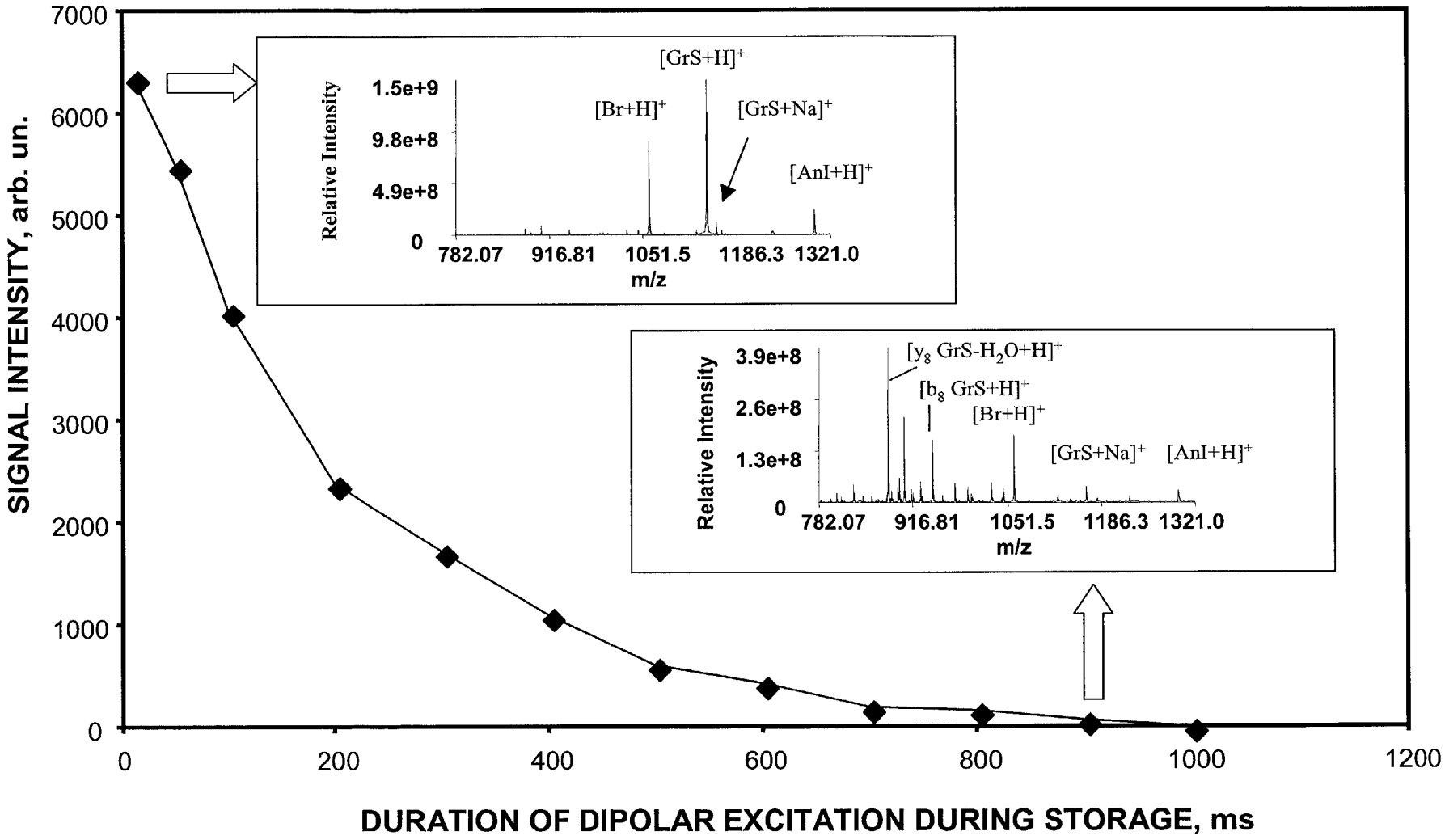

gramicidin S [GrS+H]+
angiotensin I [AnI+H]+
INTENSITY OF [GrS+H]+, arb.un.
INTENSITY OF [AnI+H]+, arb.un.
FREQUENCY, kHz
0
200
400
600
800
1000
1200
1400
0
20
40
60
80
100
120
60
70
80
90
100
110
120
130

FIGURE 5


SIGNAL INTENSITY, arb. un.
7000
6000
5000
4000
3000
2000
1000
0
0
200
400
600
800
1000
1200
DURATION OF DIPOLAR EXCITATION DURING STORAGE, ms
Relative Intensity
1.5e+9
9.8e+8
4.9e+8
0
[GrS+H]+
[Br+H]+
[GrS+Na]+
[AnI+H]+
782.07
916.81
1051.5
1186.3
1321.0
m/z
Relative Intensity
3.9e+8
2.6e+8
1.3e+8
0
[y8 GrS-H2O+H]+
[b8 GrS+H]+
[Br+H]+
[GrS+Na]+
[AnI+H]+
782.07
916.81
1051.5
1186.3
1321.0
m/z

TO2TOT" 5059766D

FIGURE 6

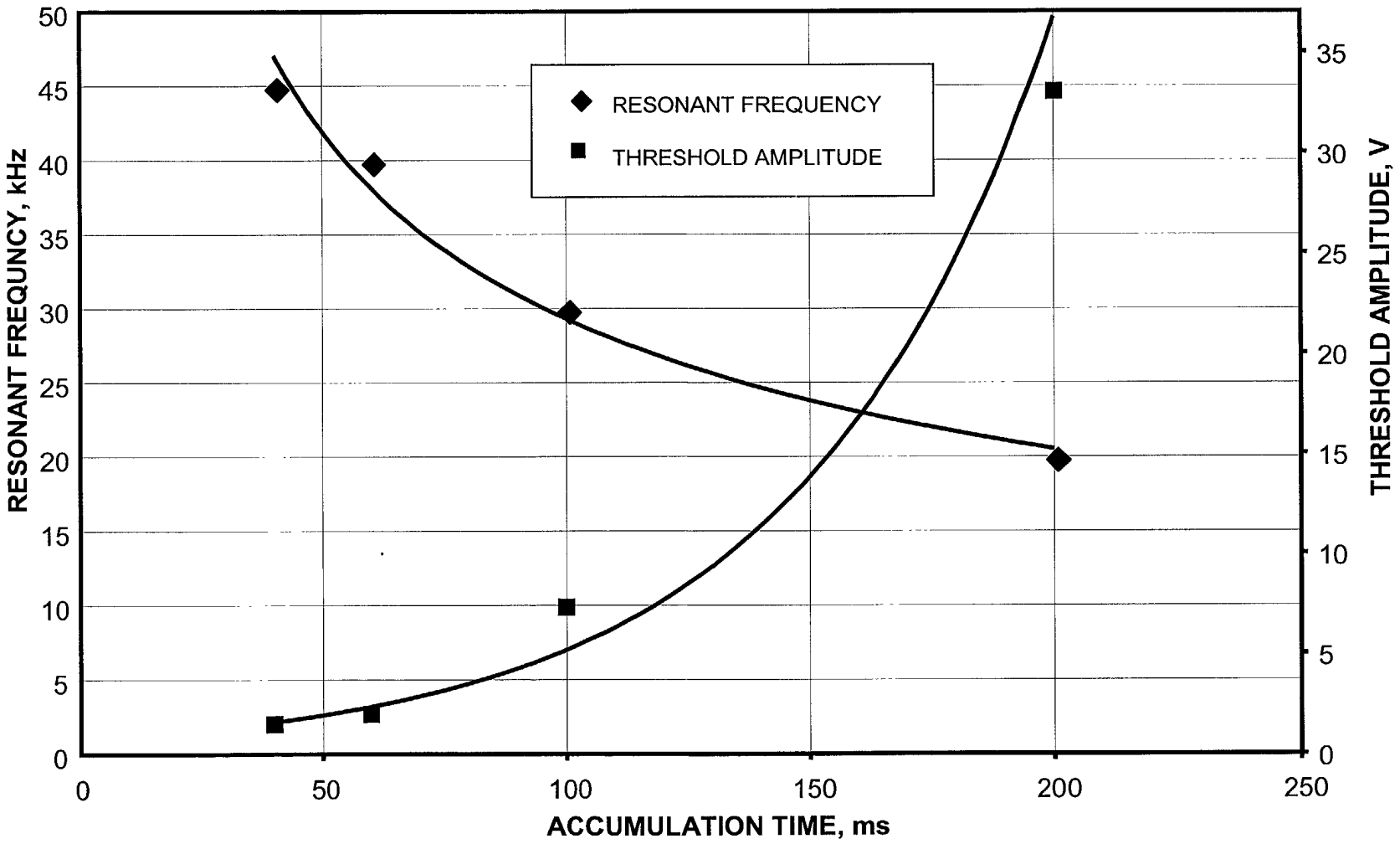
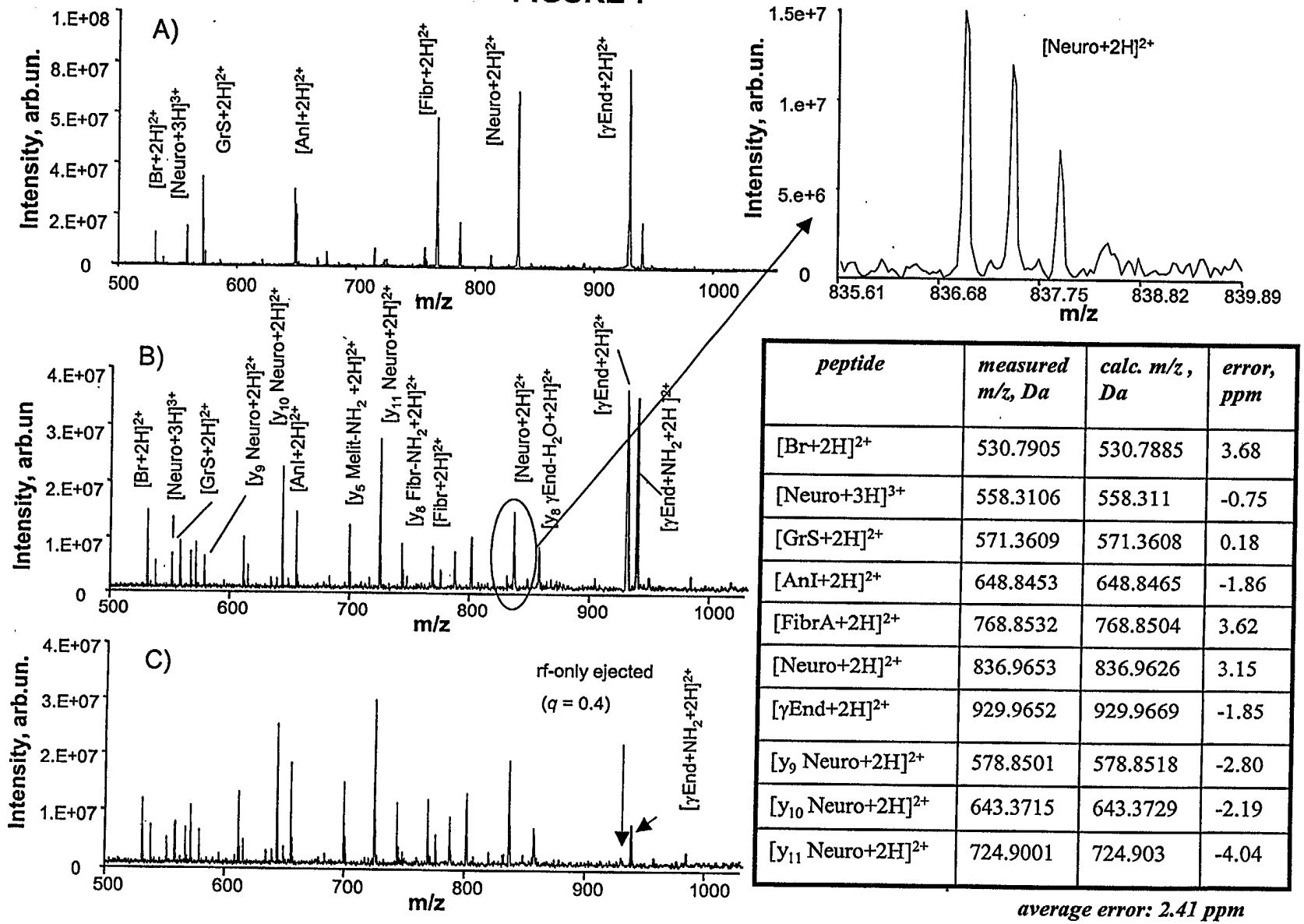


FIGURE 7



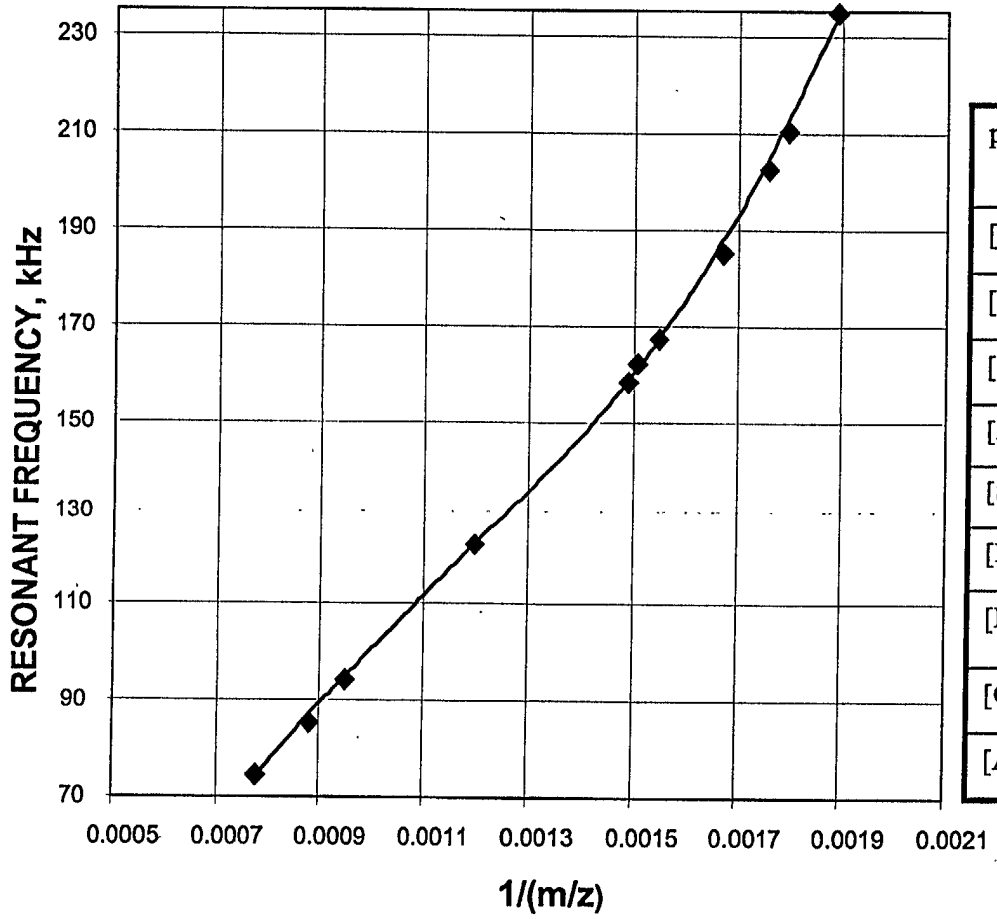
peptide	*measured m/z, Da*	*calc. m/z , Da*	*error, ppm*
$[Br+2H]^{2+}$	530.7905	530.7885	3.68
$[Neuro+3H]^{3+}$	558.3106	558.311	-0.75
$[GrS+2H]^{2+}$	571.3609	571.3608	0.18
$[AnI+2H]^{2+}$	648.8453	648.8465	-1.86
$[FibrA+2H]^{2+}$	768.8532	768.8504	3.62
$[Neuro+2H]^{2+}$	836.9653	836.9626	3.15
$[\gamma End+2H]^{2+}$	929.9652	929.9669	-1.85
$[y_9$ Neuro$+2H]^{2+}$	578.8501	578.8518	-2.80
$[y_{10}$ Neuro$+2H]^{2+}$	643.3715	643.3729	-2.19
$[y_{11}$ Neuro$+2H]^{2+}$	724.9001	724.903	-4.04

average error: 2.41 ppm

T03T0T' 5059660

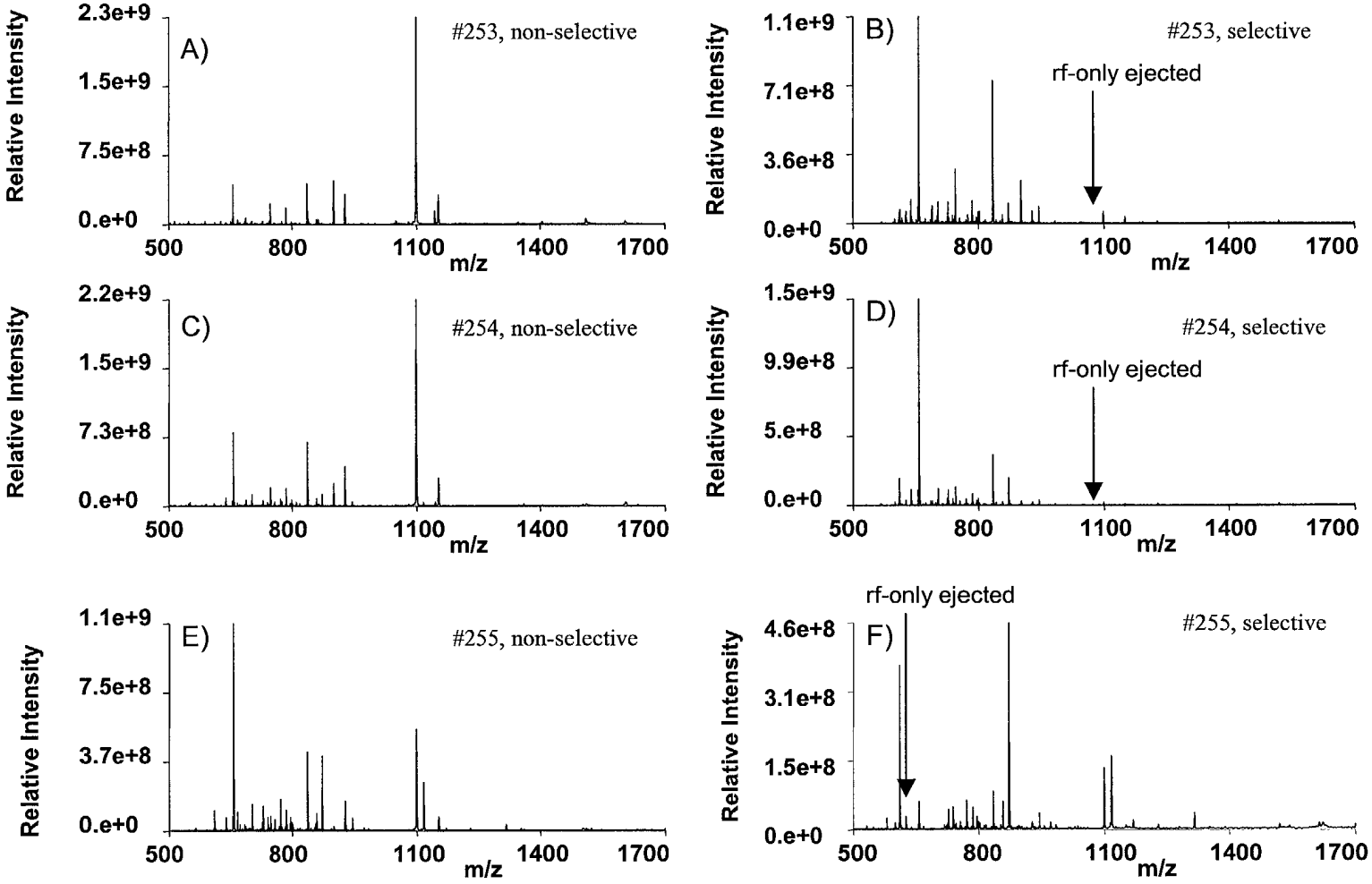
FIGURE 8

$f_{interpol}(Hz) = 7.009470x10^{13}x(1/m/z)^3+2.299154x10^{11}x(1/m/z)^2+3.614403x10^8x(1/m/z)+1.007772x10^5$



peptide	f_{exper}(Hz), experiment	$f_{predict}$(Hz), predicted	Maximum resolution
$[Br+2H]^{2+}$	234500	232773.47	135
$[Neuro+3H]^{3+}$	210500	211722.22	172
$[GrS+2H]^{2+}$	202500	203511.93	200
$[AnI+2H]^{2+}$	167500	166711.62	212
$[SubP+2H]^{2+}$	158500	158145.75	447
$[Neuro+2H]^{2+}$	122500	122390.09	1114
$[Br+H]^{+}$	94000	94334.15	280
$[GrS+H]^{+}$	85000	86457.77	58
$[AngI+H]^{+}$	74500	73330.01	64

FIGURE 9


A)
#253, non-selective
B)
#253, selective
rf-only ejected
C)
#254, non-selective
D)
#254, selective
rf-only ejected
E)
#255, non-selective
F)
#255, selective
rf-only ejected
Relative Intensity
m/z
2.3e+9
1.5e+9
7.5e+8
0.e+0
1.1e+9
7.1e+8
3.6e+8
2.2e+9
1.5e+9
7.3e+8
1.5e+9
9.9e+8
5.e+8
1.1e+9
7.5e+8
3.7e+8
4.6e+8
3.1e+8
1.5e+8
500
800
1100
1400
1700